Supporting Information

Modulation of Excimer Formation of 9-(dicyano-vinyl)julolidine by the Macrocyclic Hosts

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Parameters	α-CD-	β-CD-	γ-CD-DCVJ		
(kcal/mol)	DCVJ(1:1)	DCVJ(1:1)	1:1	1:2	2:2
Binding Energy	-8.11	-5.47	-6.84	-8.92	-11.77
Intermolecular Energy	-8.4	-5.72	-7.14	-9.21	-12.06
vdW-hb desolvation energy	-8.44	-5.82	-7.12	-9.16	-12.01
Electrostatic Energy	0.03	0.1	-0.02	-0.06	-0.06
Total internal energy	-0.24	-0.28	-0.30	0.00	0.00
Tortional energy	0.30	0.30	0.30	0.00	0.00
Unbound energy	-0.24	-0.28	-0.30	0.00	0.00



Figure S1: Concentration dependent (a) absorption and (b) emission spectra of DCVJ in pH 7 buffer.

<u>Note 1</u>:

The excitation spectra recorded for DCVJ at lower γ -CD concentration (<3mM) shows a single band at ~460 nm and a small hump at ~440 nm (Figure S2 and Figure S3). However, at a relatively higher concentration (~6 mM) a new band appeared at ~440 nm. Since the new band is absent in case of β -CD even at higher concentration, it supports the formation of 1:2 inclusion complex between dye and γ -CD. Moreover, the excitation spectra of DCVJ at very high γ -CD concentration (>10mM) differ from that of lower γ -CD concentration (Figure S2 and Figure S3). It indicates that the inclusion complex formed at higher concentration is distinct from that of lower concentration, and it supports our hypothesis that 2:2 host-guest inclusion complex is formed at higher γ -CD concentration.



Figure S2: Excitation spectra of DCVJ monitored at 515 nm in presence of (a) α -CD, (b) β -CD and (c) γ -CD.



Figure S3: Excitation spectra of DCVJ monitored at 575nm in presence of (a) α -CD, (b) β -CD and (c) γ -CD.



Figure S4: Benesi-Hildebrand plot of DCVJ:γ-CD (2:2) complex formation monitored at 575 nm.



Figure S5: Docked complex (1:1) of α -CD-DCVJ. (a) and (b) correspond to the different orientations of the same docked complex. DCVJ is shown in ball and stick model (orange) and CD is shown in stick model (element based color) and surface representation (blue color).



Figure S6: Docked complex (1:1) of β -CD-DCVJ. (a) and (b) correspond to the different orientations of the same docked complex. Rest is same as that of Figure S5.



Figure S7: Docked complex (1:1) of γ -CD-DCVJ. (a) and (b) correspond to the different orientations of the same docked complex. Rest is same as that of Figure S5.



Figure S8: Docked structures of γ -CD-DCVJ (1:2) inclusion complex. DCVJs are shown in green and orange colors with ball and stick model. (a), (b) correspond to the different orientations of the same docked complex.



Figure S9: Docked structures of γ -CD-DCVJ (2:2) inclusion complex. Rest is same as that of Figure S8.